

Diethyl sulfate

64-67-5 | DTXSID1024045

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 6.95e-01

Global applicability domain: Inside

Local applicability domain index: 4.58e-01

Confidence level: 3.90e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Diethyl sulfate</div> <div>Measured: 1.14</div> <div>Predicted: 6.95e-01</div>	<div>Image not found</div> <div>Propylene carbonate</div> <div>Measured: -0.410</div> <div>Predicted: -0.274</div>	<div>Image not found</div> <div>Trimethyl phosphate</div> <div>Measured: -0.650</div> <div>Predicted: -0.414</div>
<div>Image not found</div> <div>Fosetyl</div> <div>Measured: -2.70</div> <div>Predicted: -2.12</div>	<div>Image not found</div> <div>Triethyl phosphate</div> <div>Measured: 0.8</div> <div>Predicted: 8.20e-01</div>	